Optimization-Based Transport of Passive Tracers

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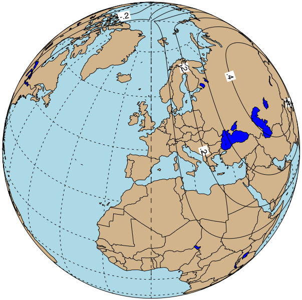
Motivation

Tracers in atmospheric modeling

- Typically tracers are chemical species transported with the flow
- In current atmospheric dynamical cores tracer advection accounts for 50% of total cost with 26 tracers
- More detailed biogeochemistry requires 100-1000 tracers



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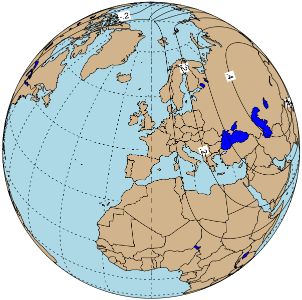
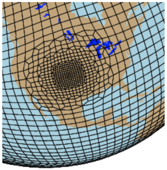


Objective:

- Develop computationally efficent tracer advection algorithms that
  - enforce physical tracer bounds
  - exploit the fact that we will be transporting hundreds of species
  - work on unstructured grids



Transport Problem

A tracer, represented by its mixing ratio q and mass ρq, is transported in the flow with velocity $\mathbf{u}$

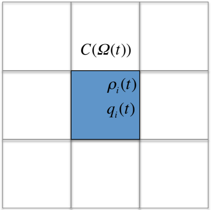
$$\left.\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \\ \frac{\partial \rho q}{\partial t} + \nabla \cdot \rho q \mathbf{u} = 0 \end{aligned}\right\} \rightarrow \frac{Dq}{Dt} = 0$$

Solution methods should satisfy

- conservation of ρq
- monotonicity or bounds preservation of q
- consistency between q and ρ (free stream preserving)
- preservation of linear correlations between tracers ($q_1 = a q_2 + b$)

Incremental Remap for Transport

Given a partition $C(\Omega)$ *into cells* $c_i, i = 1, ...C$



- cell mass $m_i = \int_{c_i} \rho(\mathbf{x}, t) dV$
- cell area $\mu_i = \int_{c_i} dV$
- cell average density $\rho_i = \dfrac{m_i}{\mu_i}$
- cell average tracer concentration

$$q_i = \frac{\int_{c_i} \rho(\mathbf{x}, t) q(\mathbf{x}, t) dV}{\int_{c_i} \rho(\mathbf{x}, t) dV}$$

$$\int_{c_i} \rho(\mathbf{x}, t) q(\mathbf{x}, t) dV = m_i q_i$$

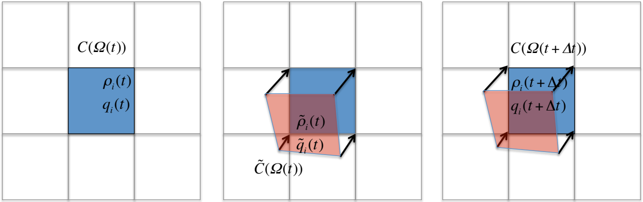
Dukowicz and Baumgardner (2000) *JCP*

For a Lagrangian volume, V_L

$$\frac{d}{dt} \int_{V_L} \rho(\mathbf{x}, t) dV = 0$$

$$\frac{d}{dt} \int_{V_L} q(\mathbf{x}, t) \rho(\mathbf{x}, t) dV = 0$$

Incremental Remap for Transport



1. Project arrival grid to departure grid: $C(\Omega(t+\Delta t)) \mapsto \widetilde{C}(\Omega(t))$
2. Remap: $\rho(t) \mapsto \tilde{\rho}(t)$, $q(t) \mapsto \widetilde{q}(t)$
3. Lagrangian update:

$$m_i(t+\Delta t) = \tilde{m}_i(t), \quad \rho_i(t+\Delta t) = \frac{m_i(t+\Delta t)}{\mu_i(t+\Delta t)}, \quad q_i(t+\Delta t) = \tilde{q}_i(t)$$

Dukowicz and Baumgardner (2000) *JCP*

Density and Tracer Remap

Given mean density and tracer values ρ_i, q_i on the *old* grid cells c_i, find accurate approximations for $\widetilde{m}_i$ and $\widetilde{q}_i$ on the *new* cells $\widetilde{c}_i$ such that:

- Total mass and tracer mass are conserved:

$$\sum_{i=1}^{C} \widetilde{m}_i = \sum_{i=1}^{C} m_i = M \qquad \sum_{i=1}^{C} \widetilde{m}_i \widetilde{q}_i = \sum_{i=1}^{C} m_i q_i = Q\,.$$

- Mean density and tracer approximations on the new cells, $\widetilde{\rho}_i = \frac{\widetilde{m}_i}{\widetilde{\mu}_i}$ and $\widetilde{q}_i$ satisfy the local bounds

$$\rho_i^{\text{min}} \le \widetilde{\rho}_i \le \rho_i^{\text{max}}\,, \quad i = 1, \ldots, C\,,$$

$$q_i^{\text{min}} \le \widetilde{q}_i \le q_i^{\text{max}}\,, \quad i = 1, \ldots, C\,,$$

Optimization-Based Remap

Objective

$$\|\widetilde{u} - u^T\|$$

minimize the distance between the solution and a suitable target

Target

$$\partial_t u^{\mathsf{T}} = L^h u^{\mathsf{T}}$$

stable and accurate solution, not required to possess all desired physical properties

Constraints

$$\underline{C} \leq C\widetilde{u} \leq \overline{C}$$

desired physical properties viewed as constraints on the state

Advantages

- Solution is globally optimal with respect to the target and desired physical properties
- Decouples accuracy from enforcement of physical properties

Bochev, Ridzal, Shashkov (2013) *JCP*

Density Formulation

$$
\begin{aligned}
\widetilde{m}_i &= \int_{c_i} \rho(\boldsymbol{x})dV &+& \left(\int_{\widetilde{c}_i} \rho(\boldsymbol{x})dV - \int_{c_i} \rho(\boldsymbol{x})dV\right) \\
&= \quad m_i &+& \quad u_i
\end{aligned}
$$

- *Objective* $\frac{1}{2}\|\widetilde{u} - u^{\mathsf{T}}\|_{\ell_2}^2$
- *Target* $u_i^{\mathsf{T}} := \displaystyle\int_{\widetilde{c}_i} \rho^h(\boldsymbol{x})dV - \int_{c_i} \rho^h(\boldsymbol{x})dV$
- *Constraints* $\displaystyle\sum_{i=1}^{C} \widetilde{u}_i = 0, \quad \rho_i^{min}\widetilde{\mu}_i \leq \widetilde{m}_i \leq \rho_i^{max}\widetilde{\mu}_i$

Bochev, Ridzal, Shashkov (2013) *JCP*

Tracer Formulation

$$\widetilde{q}_i = \frac{\int_{\widetilde{c}_i} \rho(\boldsymbol{x}) q(\boldsymbol{x}) dV}{\int_{\widetilde{c}_i} \rho(\boldsymbol{x}) dV}$$

- *Objective* $\frac{1}{2} \|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2$
- *Target* $q_i^{\mathsf{T}} := \frac{\int_{\widetilde{c}_i} \rho^h(\boldsymbol{x}) q^h(\boldsymbol{x}) dV}{\int_{\widetilde{c}_i} \rho^h(\boldsymbol{x}) dV}$
- *Constraints* $\sum_{i=1}^{C} \widetilde{m}_i \widetilde{q}_i = Q, \quad q_i^{min} \leq \widetilde{q}_i \leq q_i^{max}$

OBR Algorithm

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{u} - u^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{C} \widetilde{u}_i = 0, \quad m_i^{\text{min}} \le m_i + \widetilde{u}_i \le m_i^{\text{max}} \end{cases}$$

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{C} \widetilde{m}_i \widetilde{q}_i = Q, \quad q_i^{\text{min}} \le \widetilde{q}_i \le q_i^{\text{max}} \end{cases}$$

Singly linearly constrained quadratic programs with simple bounds

- Solve related separable problem (without mass constraint) first, cost $O(C)$
- Satisfy the mass conservation constraint in a few secant iterations

Density and Tracer Reconstructions

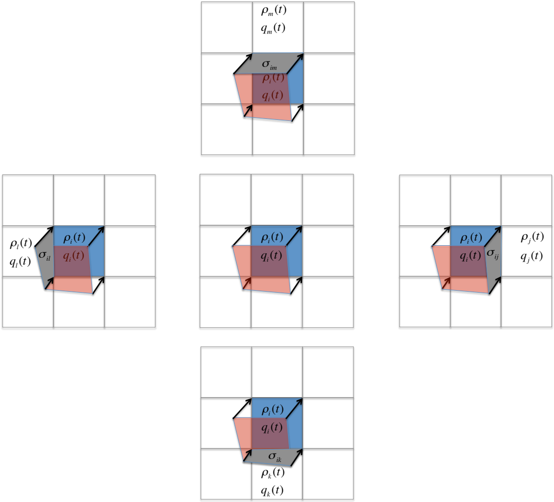
$$\rho^h(\mathbf{x})|_{c_i} = \rho_i + \mathbf{g}_i^\rho \cdot (\mathbf{x} - \mathbf{b}_i)$$

$$q^h(\mathbf{x})|_{c_i} = q_i + \mathbf{g}_i^q \cdot (\mathbf{x} - \mathbf{c}_i)$$

- Approximate gradients ($\mathbf{g}_i^\rho \approx \nabla\rho$, $\mathbf{g}_i^q \approx \nabla q$) computed using least-squares fit with five point stencil
- Cell barycenter $\mathbf{b}_i = \dfrac{\int_{c_i} \mathbf{x}\, dV}{\mu_i}$
- Cell center of mass $\mathbf{c}_i = \dfrac{\int_{c_i} \mathbf{x}\rho_i(\mathbf{x})\, dV}{m_i}$
- Mean preserving by construction

$$\frac{1}{\mu_i}\int_{c_i} \rho^h(\mathbf{x})\, dV = \rho_i \qquad \frac{1}{m_i}\int_{c_i} \rho^h(\mathbf{x}) q^h(\mathbf{x})\, dV = q_i$$

Swept Area Approximation



$$F_{is}^{\rho} = \int_{\sigma_{is}} \rho_{i/s}^{h}(\boldsymbol{x})dV$$

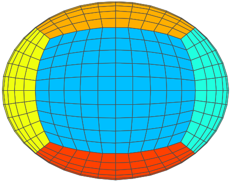
$$F_{is}^{q} = \int_{\sigma_{is}} \rho_{i/s}^{h}(\boldsymbol{x})q_{i/s}^{h}(\boldsymbol{x})dV$$

$$u_i^{\mathsf{T}} \approx \sum_s F_{is}^{\rho}$$

$$q_i^{\mathsf{T}} \approx \frac{q_i(t)m_i(t) + \sum_s F_{is}^{q}}{m_i(t) + u_i^{\mathsf{T}}}$$

Cubed Sphere Grid

- Six faces of cube projected onto surface of sphere
- Equiangular gnomonic projection with central angles, $\alpha, \beta \in [-\pi/4, \pi/4]$
- Local coordinates
  $x = a \tan\alpha, y = a \tan\beta \quad p = 1, \ldots, 6$

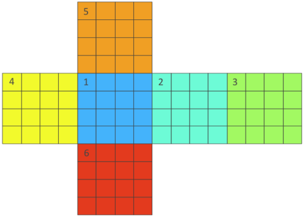


$$\int_V dV = -\int_{\partial V} \frac{1}{1+x^2}\frac{y}{r}dx$$

$$\int_V x dV = -\int_{\partial V} \frac{1}{1+x^2}\frac{xy}{r}dx$$

$$\int_V y dV = \int_{\partial V} \frac{1}{r}dx$$

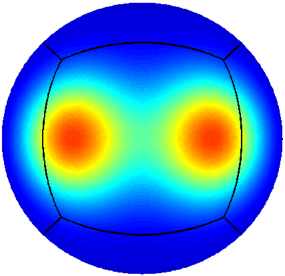
$$r = \sqrt{1+x^2+y^2} \text{ for } a = 1$$



See Ullrich *et al.* (2009) Monthly Weather Review, Lauritzen *et al.*(2010) JCP.

Convergence Test - Solid Body Rotation

- Initial density distribution set to one everywhere
- Initial tracer distribution two smooth Gaussian hills centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent rotational flow field, $\alpha = \pi/4$:

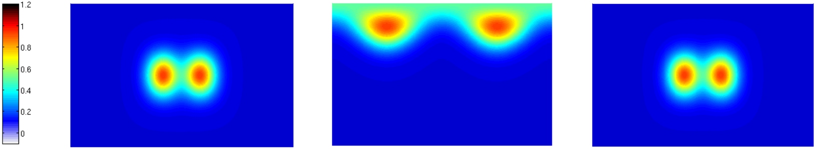


$$u(\lambda, \theta) = 2\pi \left(\cos(\theta)\cos(\alpha) + \cos(\lambda)\sin(\theta)\sin(\alpha)\right)$$

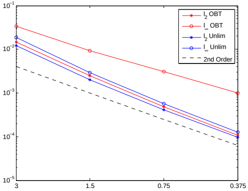
$$v(\lambda, \theta) = 2\pi \sin(\lambda)\sin(\alpha)$$

Convergence Test - Solid Body Rotation

$t = 0$ | $t = 2.5$ | $t = 5$



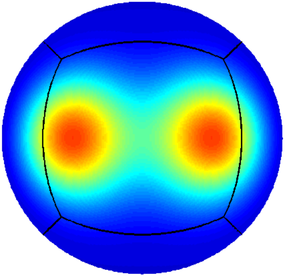
		OBT*		Unlimited	
mesh	steps	l_2	l_∞	l_2	l_∞
3.0°	600	0.0145	0.0338	0.0120	0.0185
1.5°	1200	0.00247	0.00934	0.00203	0.00296
0.75°	2400	0.000486	0.00308	0.000412	0.000412
0.375°	4800	0.000108	0.000997	0.0000958	0.000127
	Rate	*2.36*	*1.69*	*2.32*	*2.39*



* Optimization-based transport

Convergence Test - Deformational Flow

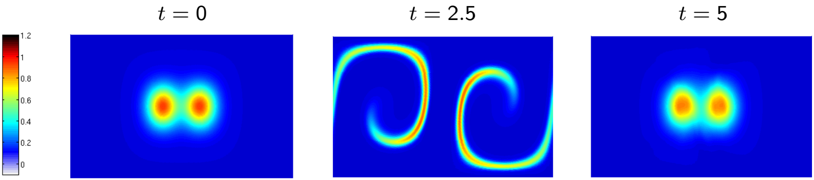
- Initial density distribution set to one everywhere
- Initial tracer distribution two smooth Guassian hills centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent deformational flow field, $T = 5$:



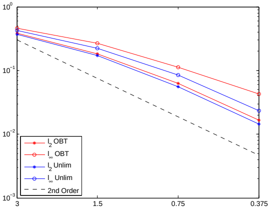
$$u(\lambda, \theta, t) = 2\sin^2(\lambda - 2\pi t/T)\sin(2\theta)\cos(\pi t/T) + 2\pi\cos(\theta)/T$$

$$v(\lambda, \theta, t) = 2\sin(2(\lambda - 2\pi t/T))\cos(\theta)\cos(\pi t/T)$$

Convergence Test - Deformational Flow



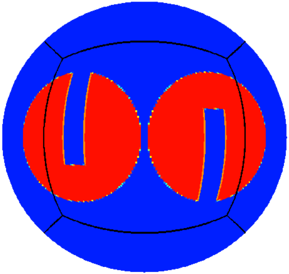
		OBT*		Unlimited	
mesh	steps	l_2	l_∞	l_2	l_∞
3.0°	600	0.386	0.465	0.368	0.425
1.5°	1200	0.182	0.268	0.172	0.225
0.75°	2400	0.0626	0.113	0.0559	0.0843
0.375°	4800	0.0167	0.0425	0.0144	0.0233
	Rate	*1.51*	*1.16*	*1.56*	*1.40*



* Optimization-based transport

Discontinuous Tracer Test

- Initial density distribution set to one everywhere
- Initial tracer distribution two notched cylinders centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent deformational flow field, $T = 5$:

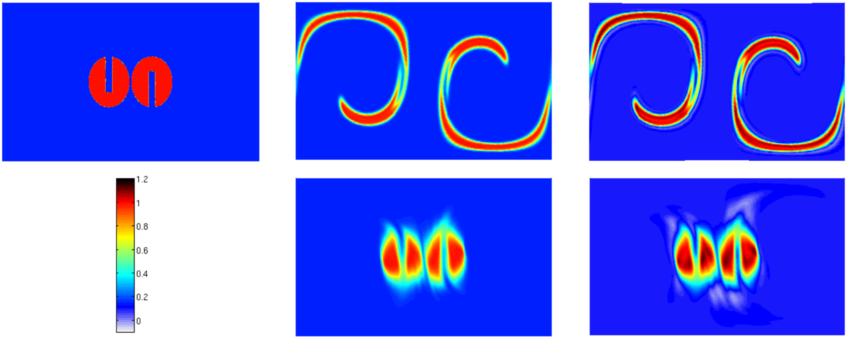


$$u(\lambda, \theta, t) = 2\sin^2(\lambda - 2\pi t/T)\sin(2\theta)\cos(\pi t/T) + 2\pi\cos(\theta)/T$$

$$v(\lambda, \theta, t) = 2\sin(2(\lambda - 2\pi t/T))\cos(\theta)\cos(\pi t/T)$$

Discontinuous Tracer Test

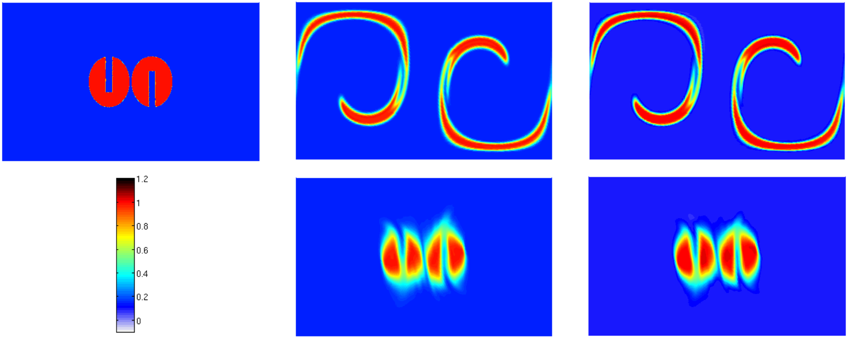
Initial | OBT | Unlimited



Initial	OBT	Unlimited
min = 0.1	min = 0.10	min = -0.020
max = 1.0	max = 1.00	max = 1.14

Discontinuous Tracer Test

Initial | OBT | Slope Limited

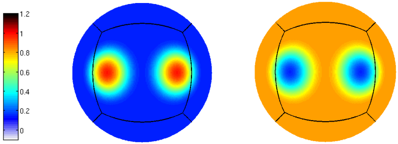


Initial	OBT	Slope Limited
min = 0.1	min = 0.10	min = 0.078
max = 1.0	max = 1.00	max = 1.030

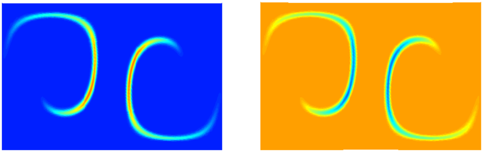
Linear Tracer Correlation Test

- Initial density distribution set to one
- Initial tracer distributions two cosine bells centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- q_1 has min = 0.1 and max = 1.0
- $q_2 = -0.8q_1 + 0.9$
- Nondivergent deformational flow

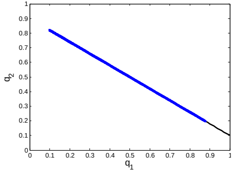
q_1 q_2



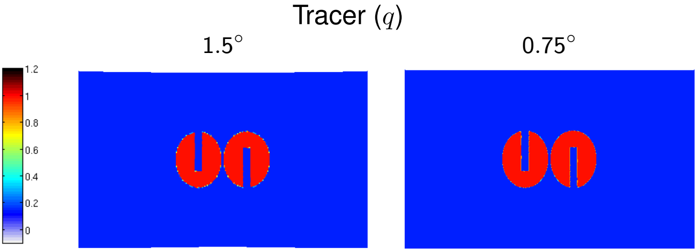
q_1 q_2

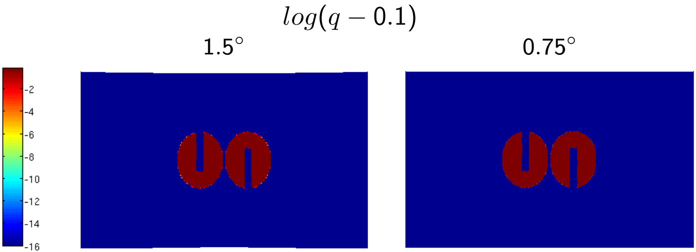


Correlation at $t = 2.5$



Locality Test - Initial Conditions

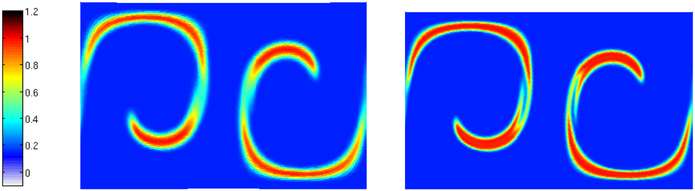




Locality Test - Deformational Flow

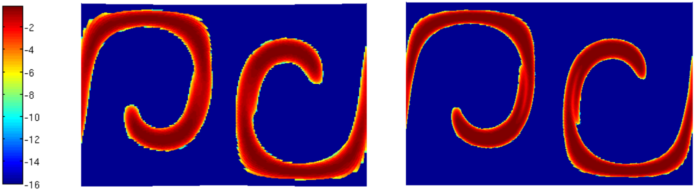
Tracer (q)

1.5°　　　　0.75°



$log(q - 0.1)$

1.5°　　　　0.75°



Locality Test - Deformational Flow

Tracer (q)

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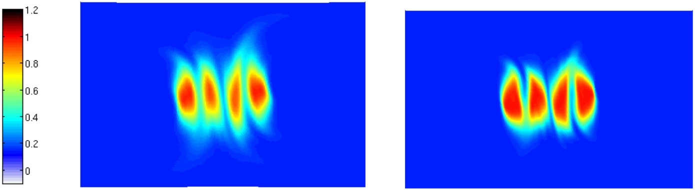
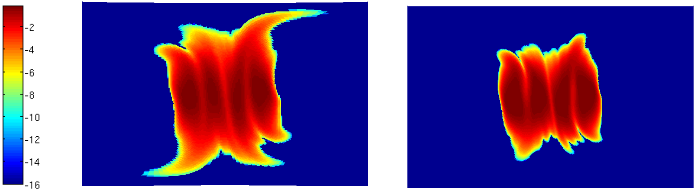


$log(q - 0.1)$

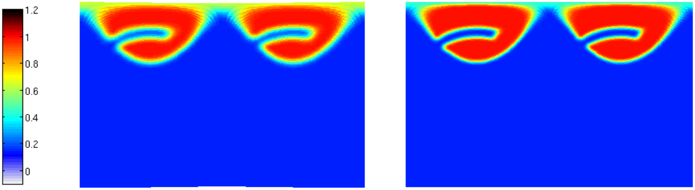
1.5°　　　　0.75°



Locality Test - Solid Body Rotation

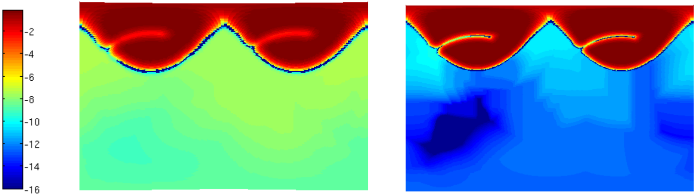
Tracer (q)

1.5°　　　　0.75°

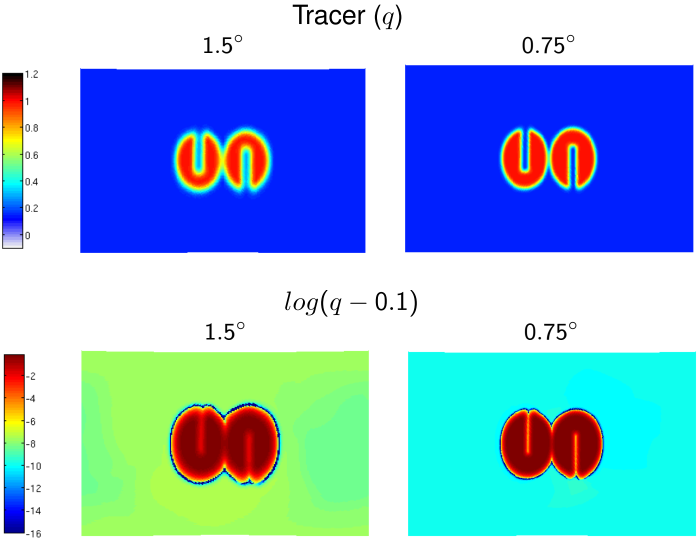


$log(q - 0.1)$

1.5°　　　　0.75°



Locality Test - Solid Body Rotation



Conclusions

- Optimization-based transport using incremental remapping offers a robust and flexible alternative to standard transport techniques
  - Solution is globally mass conserving and bounds preserving
  - Optimization algorithm is efficient and computationally competitive with standard slope limiting
  - Swept area integrals are computed once per time step are used for multiple tracers
- Future work
  - Continue to investigate the behavior of algorithm in regards to global versus local mass conservation
  - Developing optimization-based limiting for nodal spectral element semi-Lagrangian tracer transport